

10/581,034

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LOGINID: ssspta1201txs

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

NEWS 1 Web Page for STN Seminar Schedule - N. America  
NEWS 2 MAY 01 New CAS web site launched  
NEWS 3 MAY 08 CA/CAplus Indian patent publication number format defined  
NEWS 4 MAY 14 RDISCLOSURE on STN Easy enhanced with new search and display  
NEWS 5 MAY 21 fields  
BIOSIS reloaded and enhanced with archival data  
NEWS 6 MAY 21 TOXCENTER enhanced with BIOSIS reload  
NEWS 7 MAY 21 CA/CAplus enhanced with additional kind codes for German patents  
NEWS 8 MAY 22 CA/CAplus enhanced with IPC reclassification in Japanese patents  
NEWS 9 JUN 27 CA/CAplus enhanced with pre-1967 CAS Registry Numbers  
NEWS 10 JUN 29 STN Viewer now available  
NEWS 11 JUN 29 STN Express, Version 8.2, now available  
NEWS 12 JUL 02 LEMBASE coverage updated  
NEWS 13 JUL 02 LMEDLINE coverage updated  
NEWS 14 JUL 02 SCISEARCH enhanced with complete author names  
NEWS 15 JUL 02 CHEMCATS accession numbers revised  
NEWS 16 JUL 02 CA/CAplus enhanced with utility model patents from China  
NEWS 17 JUL 16 CAplus enhanced with French and German abstracts  
NEWS 18 JUL 18 CA/CAplus patent coverage enhanced  
NEWS 19 JUL 26 USPATFULL/USPAT2 enhanced with IPC reclassification  
NEWS 20 JUL 30 USGENE now available on STN  
NEWS 21 AUG 06 CAS REGISTRY enhanced with new experimental property tags  
NEWS 22 AUG 06 BEILSTEIN updated with new compounds  
NEWS 23 AUG 06 FSTA enhanced with new thesaurus edition  
NEWS 24 AUG 13 CA/CAplus enhanced with additional kind codes for granted patents  
NEWS 25 AUG 20 CA/CAplus enhanced with CAS indexing in pre-1907 records  
NEWS 26 AUG 27 Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB  
NEWS 27 AUG 27 USPATOLD now available on STN  
NEWS 28 AUG 28 CAS REGISTRY enhanced with additional experimental spectral property data

10/581, 034

NEWS 29 SEP 07 STN AnaVist, Version 2.0, now available with Derwent World Patents Index  
NEWS 30 SEP 13 FORIS renamed to SOFIS  
NEWS 31 SEP 13 INPADOCDB: New SDI frequency MONTHLY available now  
  
NEWS EXPRESS 05 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2,  
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 05 SEPTEMBER 2007.  
  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS LOGIN Welcome Banner and News Items  
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 20:28:06 ON 14 SEP 2007

FILE 'REGISTRY' ENTERED AT 20:28:19 ON 14 SEP 2007  
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STRUCTURE FILE UPDATES: 13 SEP 2007 HIGHEST RN 947061-18-9  
DICTIONARY FILE UPDATES: 13 SEP 2007 HIGHEST RN 947061-18-9

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information

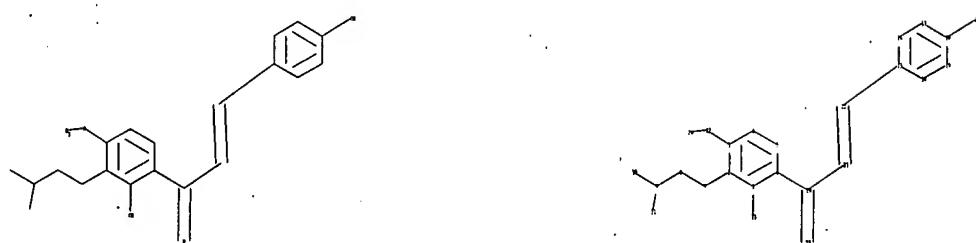
10/581,034

on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10581034.str



chain nodes :

7 8 9 10 11 12 13 20 21 22 23 24 26

ring nodes :

1 2 3 4 5 6 14 15 16 17 18 19

chain bonds :

1-13 2-7 3-12 6-20 7-8 8-9 9-10 9-11 12-26 15-22 18-24 20-21

20-23 21-22

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-19 15-16 16-17 17-18 18-19

exact/norm bonds :

1-13 3-12 12-26 18-24 20-23

exact bonds :

2-7 6-20 7-8 8-9 9-10 9-11 15-22 20-21 21-22

normalized bonds :

10/581,034

1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-19 15-16 16-17 17-18 18-19  
isolated ring systems :  
containing 1 : 14 :

G1:H,CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS  
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom  
18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS  
26:CLASS

L1 STRUCTURE UPLOADED

=> s 11  
SAMPLE SEARCH INITIATED 20:28:39 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 71 TO ITERATE

100.0% PROCESSED 71 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 915 TO 1925  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 ful  
FULL SEARCH INITIATED 20:28:46 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 1745 TO ITERATE

100.0% PROCESSED 1745 ITERATIONS 11 ANSWERS  
SEARCH TIME: 00.00.01

L3 11 SEA SSS FUL L1

=> file caplus  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
ENTRY SESSION  
FULL ESTIMATED COST 172.10 172.31

FILE 'CAPLUS' ENTERED AT 20:28:53 ON 14 SEP 2007  
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FILE COVERS 1907 - 14 Sep 2007 VOL 147 ISS 13  
FILE LAST UPDATED: 13 Sep 2007 (20070913/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 13  
L4 16 L3

=> file reg  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
SESSION  
FULL ESTIMATED COST ENTRY 2.82 175.13

FILE 'REGISTRY' ENTERED AT 20:32:17 ON 14 SEP 2007  
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STRUCTURE FILE UPDATES: 13 SEP 2007 HIGHEST RN 947061-18-9  
DICTIONARY FILE UPDATES: 13 SEP 2007 HIGHEST RN 947061-18-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

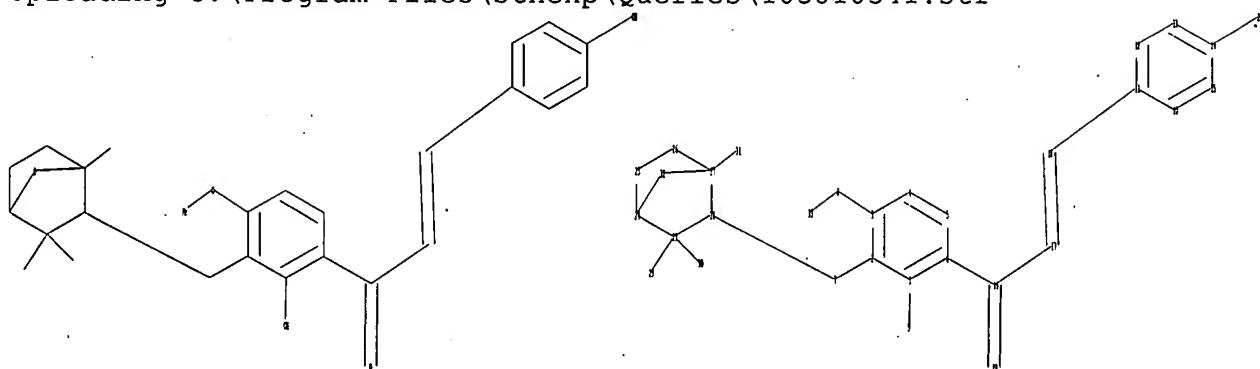
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

10/581,034

Uploading C:\Program Files\Stnexp\Queries\105810341.str



chain nodes :

7 8 9 16 17 18 19 20 29 30 31 33

ring nodes :

1 2 3 4 5 6 10 11 12 13 14 15 23 24 25 26 27 28 32

chain bonds :

1-9 2-7 3-8 6-16 7-28 8-33 11-18 14-20 16-17 16-19 17-18 23-29  
23-30 27-31

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15  
23-24 23-28 24-25 24-32 25-26 26-27 27-28 27-32

exact/norm bonds :

1-9 3-8 14-20 16-19 23-24 23-28 24-25 24-32 25-26 26-27 27-28  
27-32

exact bonds :

2-7 6-16 7-28 8-33 11-18 16-17 17-18 23-29 23-30 27-31

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15

isolated ring systems :

containing 1 : 10 :

G1:H,CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS  
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS  
18:CLASS 19:CLASS 20:CLASS 23:Atom 24:Atom 25:Atom 26:CLASS 27:Atom  
28:Atom 29:CLASS 30:CLASS 31:CLASS 6:Atom 33:CLASS

10/581,034

L5 STRUCTURE UPLOADED

=> s 15

SAMPLE SEARCH INITIATED 20:32:37 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=> s 15 ful

FULL SEARCH INITIATED 20:32:44 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 1 ANSWERS  
SEARCH TIME: 00.00.01

L7 1 SEA SSS FUL L5

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.10	347.23

FILE 'CAPLUS' ENTERED AT 20:32:51 ON 14 SEP 2007  
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FILE COVERS 1907 - 14 Sep 2007 VOL 147 ISS 13  
FILE LAST UPDATED: 13 Sep 2007 (20070913/ED)

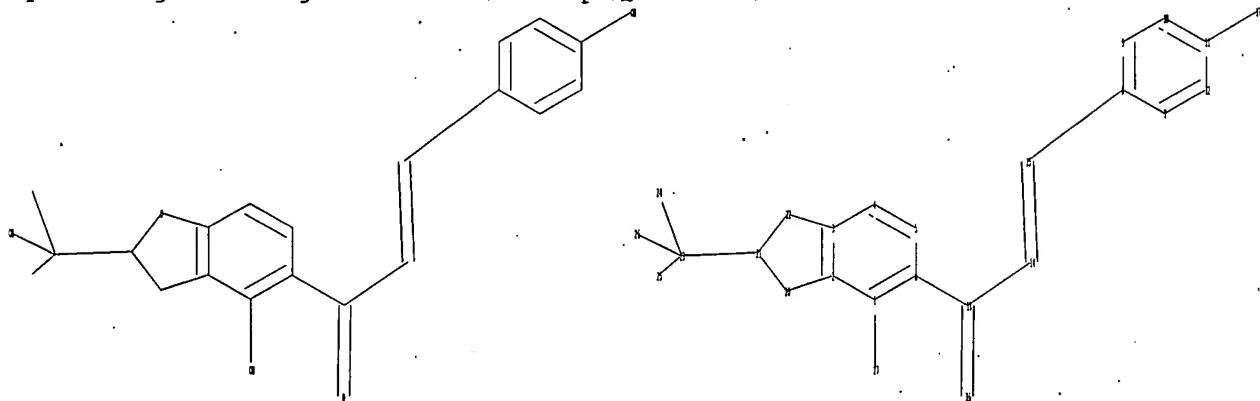
10/581,034

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They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 17  
L8            3 L7

=>  
Uploading C:\Program Files\Stnexp\Queries\105810342.str



chain nodes :  
13 14 15 16 17 23 24 25 26 27  
ring nodes :  
1 2 3 4 5 6 7 8 9 10 11 12 20 21 22  
chain bonds :  
1-27 6-13 8-15 11-17 13-14 13-16 14-15 21-23 23-24 23-25 23-26  
ring bonds :  
1-2 1-6 2-3 2-20 3-4 3-22 4-5 5-6 7-8 7-12 8-9 9-10 10-11  
11-12 20-21 21-22  
exact/norm bonds :  
1-27 11-17 13-16 23-26  
exact bonds :  
2-20 3-22 6-13 8-15 13-14 14-15 20-21 21-22 21-23 23-24 23-25  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

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isolated ring systems :  
containing 1 : 7 :

G1:H,CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom  
10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS  
20:Atom 21:Atom 22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS  
27:CLASS

L9 STRUCTURE UPLOADED

=> s 19

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 20:38:21 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 1 TO 80

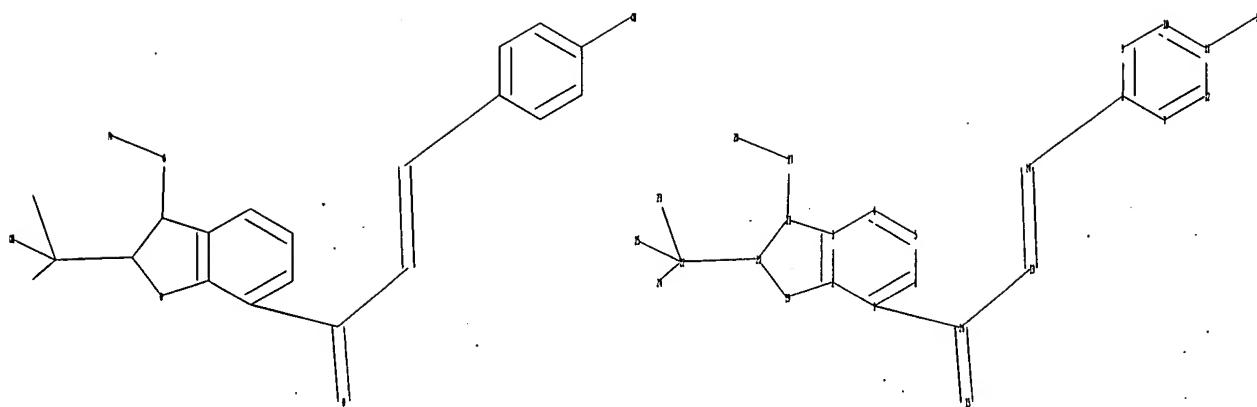
PROJECTED ANSWERS: 0 TO 0

L10 0 SEA SSS SAM L9

L11 0 L10

=>

Uploading C:\Program Files\Stnexp\Queries\105810343.str



chain nodes :

13 14 15 16 22 23 24 25 26 27 28

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 19 20 21

chain bonds :

1-26 8-14 11-16 13-14 13-26 15-26 20-22 21-27 22-23 22-24 22-25

27-28

ring bonds :

1-2 1-6 2-3 2-19 3-4 3-21 4-5 5-6 7-8 7-12 8-9 9-10 10-11

11-12 19-20 20-21

exact/norm bonds :

11-16 15-26 21-27 22-25

exact bonds :

1-26 2-19 3-21 8-14 13-14 13-26 19-20 20-21 20-22 22-23 22-24

27-28

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

isolated ring systems :

containing 1 : 7 :

G1:H,CH3

Match level :

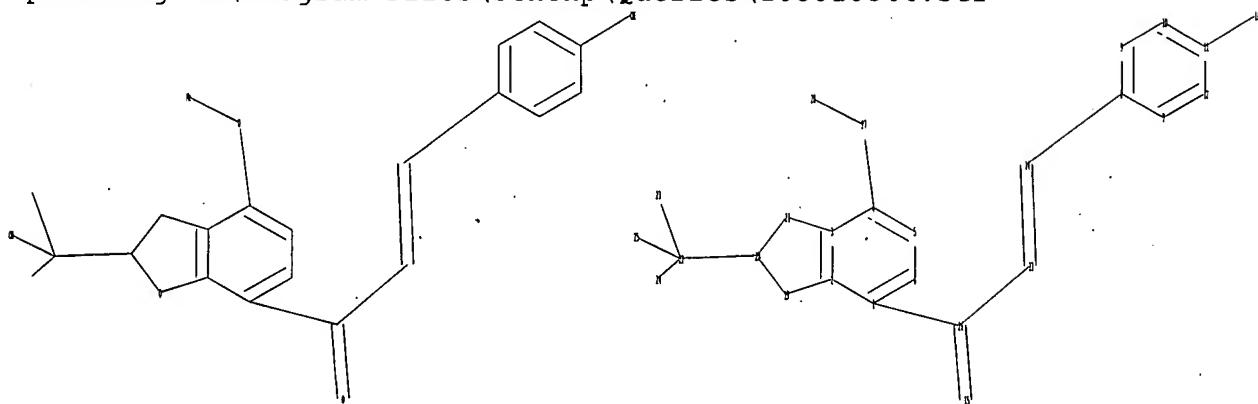
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom  
 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 19:Atom  
 20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS  
 27:CLASS 28:CLASS

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L12 STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\105810344.str



chain nodes :

13 14 15 16 22 23 24 25 26 27 28

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 19 20 21

chain bonds :

1-26 4-27 8-14 11-16 13-14 13-26 15-26 20-22 22-23 22-24 22-25

27-28

ring bonds :

1-2 1-6 2-3 2-19 3-4 3-21 4-5 5-6 7-8 7-12 8-9 9-10 10-11

11-12 19-20 20-21

exact/norm bonds :

4-27 11-16 15-26 22-25

exact bonds :

1-26 2-19 3-21 8-14 13-14 13-26 19-20 20-21 20-22 22-23 22-24

27-28

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

isolated ring systems :

10/581,034

containing 1 : 7 :

G1:H,CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom  
10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 19:Atom  
20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS  
27:CLASS 28:CLASS

L13 STRUCTURE uploaded

=> s 113

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 20:42:34 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 2 TO 124  
PROJECTED ANSWERS: 0 TO 0

L14 0 SEA SSS SAM L13

L15 0 L14

=> dup rem 14 18  
PROCESSING COMPLETED FOR L4  
PROCESSING COMPLETED FOR L8  
L16 17 DUP REM L4 L8 (2 DUPLICATES REMOVED)

=> d 116 ibib abs hitstr hitind 1-17

L16 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2007:641256 CAPLUS  
DOCUMENT NUMBER: 147:64520

TITLE: Protein kinase modulation and inflammatory response inhibition by hops and Acacia products  
 INVENTOR(S): Tripp, Matthew L.; Babish, John G.; Bland, Jeffrey; Hall, Amy Jennae; Konda, Veera; Pacioretti, Linda; Desai, Anu  
 PATENT ASSIGNEE(S): Metaproteomics, LLC, USA  
 SOURCE: PCT Int. Appl., 164pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007067812	A2	20070614	WO 2006-US47196	20061211
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
US 2007154576	A1	20070705	US 2006-636867	20061211
PRIORITY APPLN. INFO.:			US 2005-748931P	P 20051209

AB Botanical compds. to modulate kinase activity are disclosed. The compds.

and methods disclosed also inhibit expression of COX-2, inhibit synthesis of prostaglandins selectively in target cells, and inhibit inflammatory response selectively. The compns. contain at least one fraction isolated

or derived from hops or Acacia.

IT 688359-98-0, Xanthohumol H 832078-79-2, Xanthohumol G

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

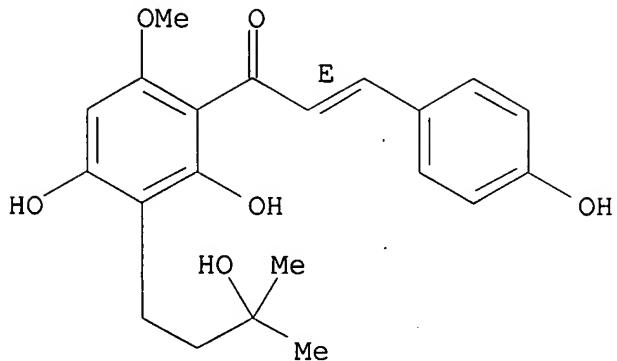
(protein kinase modulation and inflammatory response inhibition by hops

and Acacia products)

RN 688359-98-0 CAPLUS

CN 2-Propen-1-one, 1-[2,4-dihydroxy-3-(3-hydroxy-3-methylbutyl)-6-methoxyphenyl]-3-(4-hydroxyphenyl)-, (2E)- (CA INDEX NAME)

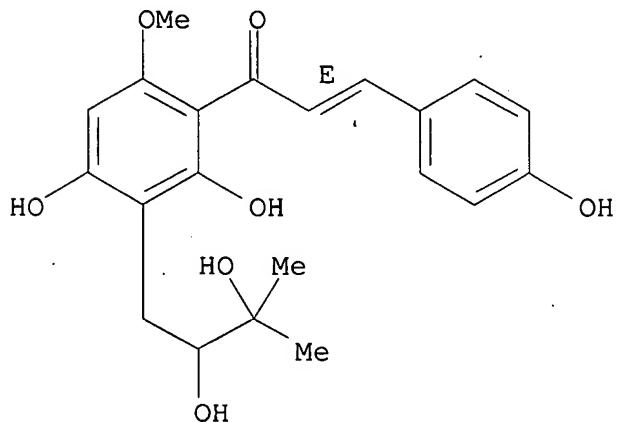
Double bond geometry as shown.



RN 832078-79-2 CAPLUS

CN 2-Propen-1-one, 1-[3-(2,3-dihydroxy-3-methylbutyl)-2,4-dihydroxy-6-methoxyphenyl]-3-(4-hydroxyphenyl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



CC 1-7 (Pharmacology)

Section cross-reference(s): 63

IT 50-81-7, Vitamin C, biological studies 94-41-7, Chalcone 94-41-7D, Chalcone, derivs. 123-08-0, 4-Hydroxybenzaldehyde 127-40-2, Lutein 144-68-3, Zeaxanthin 458-37-7, Curcumin 467-72-1, trans-Isohumulone 468-27-9, Colupulone 468-28-0, Lupulone 469-03-4, Posthumulone 474-58-8 475-36-5, Adhumulone 981-03-3, Humulinone 1406-18-4, Vitamin E 1534-03-8, cis-Isohumulone 6754-58-1, Xanthohumol 7440-50-8, Copper, biological studies 7440-66-6, Zinc, biological studies 7782-49-2, Selenium, biological studies 25269-20-9, Isocohumulone 25422-83-7, Isoadhumulone 25522-96-7, Isohumulone 26054-22-8, cis-TetrahydroIsohumulone 28374-71-2, Adlupulone 28815-20-5, Tetrahydroisohumulone 29788-67-8, trans-TetrahydroIsohumulone 34421-27-7, Tetrahydroisocohumulone 38602-23-2, CoHumulinone 52755-22-3, Hexahydrocolupulone 53846-50-7, 8-Prenylnaringenin 58501-77-2, trans-Isocohumulone 59122-94-0,

Prehumulone 65761-25-3, Prelupulone 68107-76-6, trans-Isoadhumulone  
 68127-23-1, cis-Isocohumulone 68236-11-3, 6,8-Diprenylnaringenin  
 68236-13-5, 6-Prenylnaringenin 70872-29-6, Isoxanthohumol  
 96614-01-6,  
 cis-Isoadhumulone 115063-39-3, DesmethylXanthohumol 121250-47-3,  
 Conjugatedlinoleic acid 123316-63-2, 4'-O-MethylXanthohumol  
 142628-20-4, Cohumulone 189299-03-4, 3'-Geranylchalconaringenin  
 189299-04-5, 5'-Prenylxanthohumol 189299-05-6, Xanthohumol C  
 189308-10-9, Xanthohumol B 250603-94-2, Isodehydrocycloanthohumol  
 hydrate 265659-35-6, Xanthogalenol 274266-56-7 274675-25-1,  
 Xanthohumol D 274675-26-2, Xanthohumol E 685110-34-3,  
 Hexahydroisohumulone 685110-35-4, Dihydroisohumulone 685110-36-5,  
 Tetrahydroadhumulone 685110-37-6, Hexahydroisocohumulone  
 685110-38-7,  
 Hexahydroadhumulone 688359-98-0, Xanthohumol H 688360-06-7,  
 Xanthohumol I 790664-64-1, Dihydroisocohumulone 831227-05-5,  
 Desmethylxanthohumol B 831227-06-6, Desmethylxanthohumol J  
 832078-79-2, Xanthohumol G  
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL  
 (Biological study); USES (Uses)  
 (protein kinase modulation and inflammatory response inhibition by  
 hops  
 and Acacia products)

L16 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2006:489728 CAPLUS  
 DOCUMENT NUMBER: 144:481031  
 TITLE: Carcinogenesis inhibitors containing natural  
 chalcones, coumarins, flavanones, and/or  
 diacetylene derivative  
 INVENTOR(S): Akihisa, Toshihiro; Tokuda, Harukuni; Ukiya,  
 Motohiko; Hasegawa, Daisuke  
 PATENT ASSIGNEE(S): Nihon University, Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006131594	A	20060525	JP 2004-325369	20041109
PRIORITY APPLN. INFO.:			JP 2004-325369	20041109

AB Title inhibitors contain dorsmanin A, xanthoangelol I, J, xanthotoxin,  
 isopimpinellin, ostheno, isobavachin, mundulea flavanone B,  
 8-geranylnaringenin, and/or  
 (11S,16R)-dihydroxyoctadeca-9Z,17-diene-12,14-  
 diyn-1-yl acetate. They may be added to foods, beverages, and feeds.

10/581,034

Thus, xanthoangelol I and J completely inhibited TPA-induced expression of

Epstein-Barr virus early antigen in Raji cells with their survival rate 70%, vs. 60%, for curcumin.

IT 878277-38-4P, Xanthoangelol J

RL: ADV (Adverse effect, including toxicity); FFD (Food or feed use);

NPO

(Natural product occurrence); PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)

(carcinogenesis inhibitors containing Angelica keiskei exudate constituents

with low toxicity)

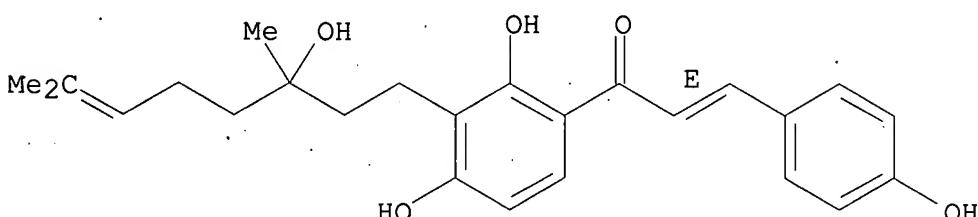
RN 878277-38-4 CAPLUS

CN 2-Propen-1-one, 1-[2,4-dihydroxy-3-(3-hydroxy-3,7-dimethyl-6-octenyl)phenyl]-3-(4-hydroxyphenyl)-, (2E)-(+)- (9CI) (CA INDEX NAME)

Rotation (+).

Double bond geometry as shown.

Currently available stereo shown.



CC 1-6 (Pharmacology)

Section cross-reference(s): 11, 17, 63

IT 298-81-7P, Xanthotoxin 482-27-9P, Isopimpinellin 484-14-0P, Osthenol

31524-62-6P, Isobavachin 87893-18-3P, 8-Geranyl naringenin

162229-27-8P, Dorsmanin A 201805-81-4P, Mundulea flavanone B

213905-35-2P, (11S,16R)-Dihydroxyoctadeca-9Z,17-diene-12,14-diyn-1-yl acetate 878277-37-3P, Xanthoangelol I 878277-38-4P, Xanthoangelol J

RL: ADV (Adverse effect, including toxicity); FFD (Food or feed use);

NPO

(Natural product occurrence); PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)

(carcinogenesis inhibitors containing Angelica keiskei exudate constituents

with low toxicity)

L16 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:35389 CAPLUS

DOCUMENT NUMBER: 144:270561

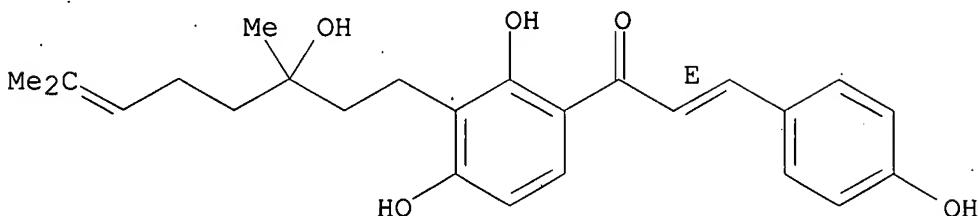
TITLE: Chalcones and Other Compounds from the Exudates of

AUTHOR(S): Angelica keiskei and Their Cancer Chemopreventive Effects  
Akihisa, Toshihiro; Tokuda, Harukuni; Hasegawa,  
Daisuke; Ukiya, Motohiko; Kimura, Yumiko; Enjo,  
Fumio;  
CORPORATE SOURCE: Suzuki, Takashi; Nishino, Hoyoku  
College of Science and Technology, Nihon  
University,  
SOURCE: Tokyo, 101-8308, Japan  
Journal of Natural Products (2006), 69(1), 38-42  
CODEN: JNPRDF; ISSN: 0163-3864  
PUBLISHER: American Chemical Society-American Society of  
Pharmacognosy  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Three new chalcones, xanthoangelol I (1), xanthoangelol J (2), and  
deoxydihydroxanthoangelol H (3), were isolated from an Et  
acetate-soluble  
fraction of exudates of the stems of Angelica keiskei, and their  
structures were established on the basis of spectroscopic methods.  
Nine aromatic compds. of known structure, 4-12, and a diacetylene, 13, were  
also isolated and identified from this same fraction. On evaluation of  
these compds. for their inhibitory effects on the induction of Epstein-Barr  
virus early antigen (EBV-EA) by 12-O-tetradecanoylphorbol-13-acetate  
(TPA)  
(TPA) in Raji cells, 1, 2, 4, and 9-12 showed potent inhibitory effects on  
EBV-EA induction. In addition, upon evaluation of the inhibitory  
effects against activation of (+)-(E)-methyl-2[(E)-hydroxyimino]-5-nitro-6-  
methoxy-3-hexamide (NOR 1), a nitrogen oxide (NO) donor, six compds.,  
namely, 1, 2, 4, 9, 11, and 12, exhibited potent inhibitory effects.  
Further, isobavachalcone (4) exhibited inhibitory effects on skin tumor  
promotion in an in vivo two-stage mouse skin carcinogenesis test using  
7,12-dimethylbenz[a]anthracene (DMBA) as an initiator and TPA as a  
promoter.  
IT 878277-38-4P, Xanthoangelol J  
RL: BSU (Biological study, unclassified); PAC (Pharmacological  
activity);  
PRP (Properties); PUR (Purification or recovery); BIOL (Biological  
study);  
PREP (Preparation)  
(isolation and characterization of chalcones and other compds. from  
the  
exudates of Angelica keiskei and their cancer chemopreventive  
effects)  
RN 878277-38-4 CAPLUS  
CN 2-Propen-1-one, 1-[2,4-dihydroxy-3-(3-hydroxy-3,7-dimethyl-6-  
octenyl)phenyl]-3-(4-hydroxyphenyl)-, (2E)-(+)- (9CI) (CA INDEX NAME)

10/581,034

Rotation (+).

Double bond geometry as shown.  
Currently available stereo shown.



CC 11-1 (Plant Biochemistry)

Section cross-reference(s): 1, 26

IT 877875-97-3P, Deoxydihydroxanthoangelol H 878277-37-3P,  
Xanthoangelol I

878277-38-4P, Xanthoangelol J

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);

PRP (Properties); PUR (Purification or recovery); BIOL (Biological study);

PREP (Preparation)

(isolation and characterization of chalcones and other compds. from the

exudates of Angelica keiskei and their cancer chemopreventive effects)

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L16 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 1

ACCESSION NUMBER: 2005:523399 CAPLUS

DOCUMENT NUMBER: 143:59727

TITLE: Extract of chalcone derivatives as aldose reductase inhibitors

INVENTOR(S): Ohnogi, Hiromu; Sugiyama, Katsumi; Enoki, Tatsuji; Kobayashi, Eiji; Sagawa, Hiroaki; Kato, Ikunoshin

PATENT ASSIGNEE(S): Takara Bio Inc., Japan

SOURCE: PCT Int. Appl., 51 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005054170	A1	20050616	WO 2004-JP17887	20041201
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,				

GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,  
 LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,  
 NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,  
 TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,  
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,  
 EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,  
 RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,  
 MR, NE, SN, TD, TG

EP 1702912 A1 20060920 EP 2004-819873 20041201

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS

CN 1890205 A 20070103 CN 2004-80036040 20041201

US 2007112066 A1 20070517 US 2006-581034 20060530

PRIORITY APPLN. INFO.: JP 2003-408215 A 20031205

WO 2004-JP17887 W 20041201

AB It is intended to provide novel chalcone compds. having carbon monoxide inhibitory effect or aldose reductase inhibitory effect, its derivs. or salts thereof. Eight chalcone derivs. were obtained from the extract of

angelica. One chalcone derivative was synthesized. These compds. showed good

inhibitory effect against aldose reductase and NO generation.

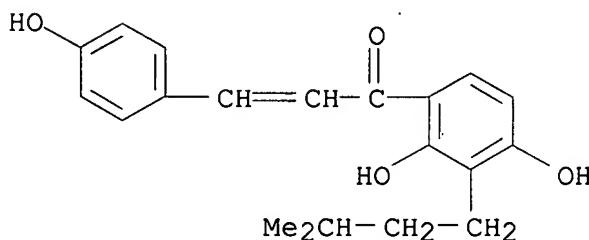
IT 853945-93-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; extract of chalcone derivs. as aldose reductase inhibitors)

RN 853945-93-4 CAPLUS

CN 2-Propen-1-one, 1-[2,4-dihydroxy-3-(3-methylbutyl)phenyl]-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



IC ICM C07C049-835

ICS C07C049-84; C07C409-08; C07D307-80; C07D493-08; A61K031-343;  
 A61K031-12; A61K031-201; A61K031-34; A61P003-10; A61P009-10;  
 A61P013-12; A61P019-02; A61P019-06; A61P019-08; A61P025-02;  
 A61P027-12; A61P029-00; A61P031-00; A61P035-00

CC 26-4 (Biomolecules and Their Synthetic Analogs)

Section cross-reference(s): 1, 17  
 IT 791112-91-9P 791112-93-1P 791112-94-2P 791112-95-3P  
 791112-96-4P  
 791112-97-5P 791632-40-1P 853945-92-3P 853945-93-4P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)  
 (drug candidate; extract of chalcone derivs. as aldose reductase  
 inhibitors)

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR  
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

L16 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2005:823550 CAPLUS  
 DOCUMENT NUMBER: 143:199938  
 TITLE: Remedy containing 3-hydroxy-3-methylglutaryl-CoA  
 reductase inhibitor and/or cell foaming inhibitor  
 INVENTOR(S): Enoki, Tatsushi; Kudo, Yoko; Sugiyama, Katsumi;  
 Ohnogi,  
 PATENT ASSIGNEE(S): Hiromu; Sagawa, Hiroaki; Kato, Ikunoshin  
 Takara Bio Inc., Japan  
 SOURCE: PCT Int. Appl., 91 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005074906	A1	20050818	WO 2005-JP1655	20050204
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: JP 2004-31173 A 20040206

OTHER SOURCE(S): MARPAT 143:199938  
 AB It is intended to provide a drug, a food, a drink or a feed for  
 treating  
 or preventing diseases, wherein an effect of inhibiting  
 3-hydroxy-3-methylglutaryl-CoA reductase and/or an effect against cell  
 foaming are needed for the prevention or treatment, characterized by

containing, as the active ingredient, at least one compound selected from the

group consisting of chalcone compds., flavanone compds., 3',4'-dihydroseseline compds., derivs. thereof and salts thereof. The above-described drug, food, drink or feed is useful in treating or preventing, for example, hyperlipemia, arteriosclerosis and various diseases caused mainly thereby. For example, xanthoangelol was isolated

from Angelica Keiskei root extract, and examined for its HMG-CoA reductase

inhibitory effect in vitro.

IT 791632-40-1P

RL: FFD (Food or feed use); NPO (Natural product occurrence); PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)

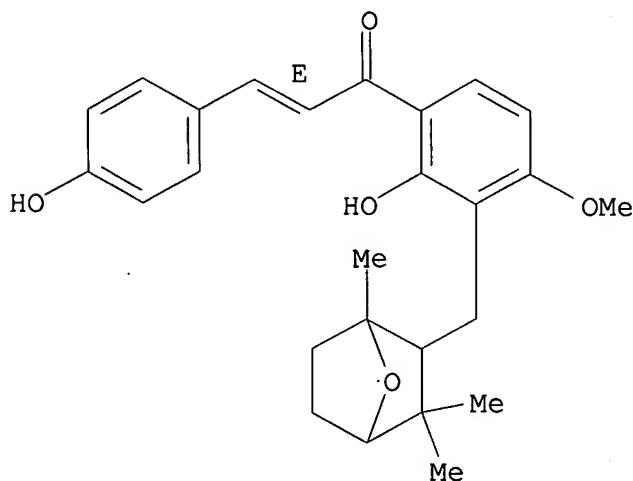
(chalcone compds., flavanone compds., and dihydroseseline compds. as 3-hydroxy-3-methylglutaryl-CoA reductase inhibitors and/or cell foaming

inhibitors)

RN 791632-40-1 CAPLUS

CN 2-Propen-1-one, 1-[2-hydroxy-4-methoxy-3-[(1,3,3-trimethyl-7-oxabicyclo[2.2.1]hept-2-yl)methyl]phenyl]-3-(4-hydroxyphenyl)-, (2E)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



IC ICM A61K031-12

ICS A23K001-16; A23L001-30; A23L002-52; A61K031-34; A61K031-343; A61K031-352; A61K031-353; A61P003-06; A61P009-10; A61P043-00; C12N009-99; C07D307-80; C07D311-32; C07D311-80; C07D493-08

CC 63-6 (Pharmaceuticals)

Section cross-reference(s): 1, 17, 18

IT 6754-58-1P, Xanthohumol 20784-50-3P, Isobavachalcone 27800-79-9P 29049-07-8P 31524-62-6P, Isobavachin 62949-76-2P, Xanthoangelol

10/581,034

160036-29-3P, 4'-O-Geranylningenin 162382-66-3P, Prostratol F  
265652-71-9P, Xanthoangelol F 265652-88-8P, Xanthoangelol G  
265652-89-9P, Xanthoangelol H 299929-45-6P 677726-10-2P  
677746-19-9P  
791112-91-9P 791112-92-0P 791112-93-1P 791112-94-2P  
791112-95-3P  
791112-96-4P 791113-21-8P 791632-40-1P 862013-04-5P  
RL: FFD (Food or feed use); NPO (Natural product occurrence); PAC  
(Pharmacological activity); PUR (Purification or recovery); THU  
(Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP  
(Preparation); USES (Uses)  
(chalcone compds., flavanone compds., and dihydroseselene compds. as  
3-hydroxy-3-methylglutaryl-CoA reductase inhibitors and/or cell  
foaming  
inhibitors)  
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR  
THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

L16 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2005:604276 CAPLUS  
DOCUMENT NUMBER: 143:259686  
TITLE: Xanthohumol Isolated from Humulus lupulus Inhibits  
Menadione-Induced DNA Damage through Induction of  
Quinone Reductase  
AUTHOR(S): Dietz, Birgit M.; Kang, Young-Hwa; Liu, Guowen;  
Eggler, Aimee L.; Yao, Ping; Chadwick, Lucas R.;  
Pauli, Guido F.; Farnsworth, Norman R.; Mesecar,  
Andrew D.; Van Breemen, Richard B.; Bolton, Judy L.  
College of Pharmacy, Department of Medicinal  
CORPORATE SOURCE: Chemistry  
and Pharmacognosy and UIC/NIH Center for Botanical  
Dietary Supplements Research, University of  
Illinois  
SOURCE: at Chicago, Chicago, IL, 60612-7231, USA  
Chemical Research in Toxicology (2005), 18(8),  
1296-1305  
CODEN: CRTOEC; ISSN: 0893-228X  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The female parts of hops (*Humulus lupulus L.*) show estrogenic effects  
as  
well as cancer chemopreventive potential. We analyzed the  
chemopreventive  
mechanism of hops by studying its antioxidative activities and its  
effect  
on the detoxification of a potentially toxic quinone (menadione). The  
detoxification enzyme quinone reductase [(NAD(P)H):quinone  
oxidoreductase,  
QR] protects against quinone-induced toxicity and has been used as a

10/581,034

marker in cancer chemoprevention studies. Although the hop extract was only

a weak quencher of free radicals formed from 1,1-diphenyl-2-picrylhydrazyl, it demonstrated strong QR induction in Hepa 1c1c7 cells.

In addition, compds. isolated from hops including xanthohumol (XH) and 8-prenyl-naringenin were tested for QR induction. Among these, XH was

the most effective at inducing QR with a concentration required to double the

specific activity of QR (CD value) of  $1.7 \pm 0.7 \mu\text{M}$ . In addition, pretreatment of Hepa1c1c7 cells with XH significantly inhibited menadione-induced DNA single-strand breaks. The QR inhibitor dicumarol reversed the protective effect of XH against menadione-induced DNA damage.

Because the expression of QR and other detoxifying enzymes is known to be

upregulated by binding of the transcription factor Nrf2 to the antioxidant

response element (ARE), the reporter activity mediated by ARE in HepG2-ARE-C8 cells was investigated after incubation with XH for 24 h. Under these conditions, XH increased ARE reporter activity in a dose-dependent manner. One mechanism by which XH might induce QR could be

through interaction with Keap1, which sequesters Nrf2 in the cytoplasm, so

that it cannot activate the ARE. Using LC-MS-MS, we demonstrated that XH

alkylates human Keap1 protein, most likely on a subset of the 27 cysteines

of Keap1. This suggests that XH induces QR by covalently modifying the Keap1 protein. Therefore, XH and hops dietary supplements might function

as chemopreventive agents, through induction of detoxification enzymes such as QR.

IT 688359-98-0, Xanthohumol H 832078-79-2, Xanthohumol G

RL: NPO (Natural product occurrence); PAC (Pharmacological activity);

THU

(Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)

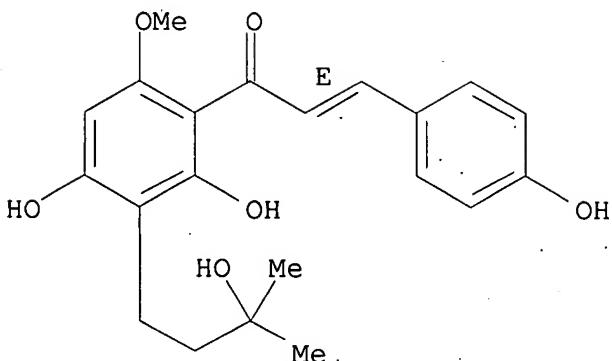
(xanthohumol from Humulus lupulus inhibits menadione-induced DNA damage

through induction of quinone reductase)

RN 688359-98-0 CAPLUS

CN 2-Propen-1-one, 1-[2,4-dihydroxy-3-(3-hydroxy-3-methylbutyl)-6-methoxyphenyl]-3-(4-hydroxyphenyl)-, (2E)- (CA INDEX NAME)

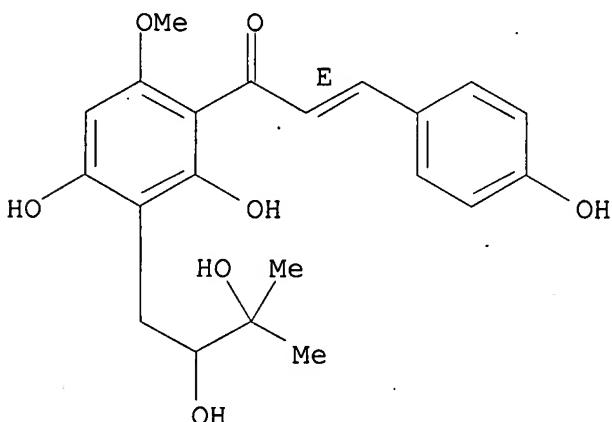
Double bond geometry as shown.



RN 832078-79-2 CAPLUS

CN 2-Propen-1-one, 1-[3-(2,3-dihydroxy-3-methylbutyl)-2,4-dihydroxy-6-methoxyphenyl]-3-(4-hydroxyphenyl)-(2E)- (CA INDEX NAME)

Double bond geometry as shown.



CC 1-6 (Pharmacology)

Section cross-reference(s): 11

IT 68236-11-3, 6,8-Diprenylnaringenin 68236-13-5, 6-Prenylnaringenin  
70872-29-6, Isoxanthohumol 189299-04-5 189299-05-6, Xanthohumol C  
189308-10-9, Xanthohumol B 274675-25-1, Xanthohumol D  
688359-98-0, Xanthohumol H 688360-06-7, Xanthohumol I  
688360-14-7 831227-04-4 831227-05-5, Desmethylxanthohumol B  
831227-06-6, Desmethylxanthohumol J 832078-79-2, Xanthohumol G  
863718-47-2

RL: NPO (Natural product occurrence); PAC (Pharmacological activity);

THU

(Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES  
(Uses)

(xanthohumol from Humulus lupulus inhibits menadione-induced DNA  
damage

through induction of quinone reductase)

REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR  
THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE.

## FORMAT

L16 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2005:602816 CAPLUS  
DOCUMENT NUMBER: 143:282488  
TITLE: In vitro antiplasmodial activity of prenylated chalcone derivatives of hops (*Humulus lupulus*) and their interaction with hemin  
AUTHOR(S): Froelich, Sonja; Schubert, Carola; Bienzle, Ulrich; Jenett-Siems, Kristina  
CORPORATE SOURCE: Institut fuer Pharmazie (Pharmazeutische Biologie), Freie Universitaet Berlin, Berlin, D-14195, Germany  
SOURCE: Journal of Antimicrobial Chemotherapy (2005), 55(6), 883-887  
PUBLISHER: CODEN: JACHDX; ISSN: 0305-7453  
Oxford University Press  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB There is an urgent need to discover new antimalarials, due to the spread of chloroquine resistance and the limited number of available drugs. Chalcones are one of the classes of natural products that are known to possess antiplasmodial properties. Therefore, the in vitro antiplasmodial activity of the main hop chalcone xanthohumol and seven derivs. was evaluated. In addition, the influence of the compds. on glutathione (GSH)-dependent hemin degradation was analyzed to determine its contribution to the antimalarial effect of chalcones. In vitro antiplasmodial activity was evaluated against the chloroquine-sensitive strain poW and the multi-resistant clone Dd2 using a [<sup>3</sup>H]hypoxanthine-incorporation assay. Inhibition of GSH-dependent hemin degradation was analyzed by a multi-well plate assay at 11  $\mu$ M. Of the eight compds. tested, four possessed activity with IC<sub>50</sub> values < 25  $\mu$ M against at least one of the two strains of *Plasmodium falciparum*. The main hop chalcone, xanthohumol, was most active with IC<sub>50</sub> values of 8.2±0.3 (poW) and 24.0±0.8  $\mu$ M (Dd2). Three of these compds. were addnl. active in the hemin-degradation assay. The results demonstrate for the first time the ability of chalcone derivs. to interfere with the hemin-degradation process of *P. falciparum*. This effect might contribute to their antiplasmodial activity. Nevertheless, as one compound showed inhibition of *P. falciparum* without being able to interact with GSH-dependent hemin degradation, other modes of action must add to the observed antiparasitic activity of hop chalcones.

10/581,034

IT 864465-61-2

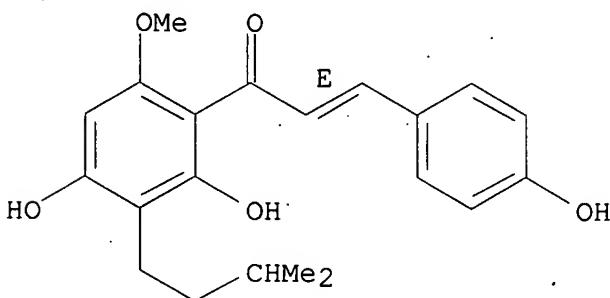
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(antiplasmoidal activity of prenylated chalcone derivs. of hops  
(Humulus lupulus) and their influence on glutathione-dependent hemin  
degradation)

RN 864465-61-2 CAPLUS

CN 2-Propen-1-one,

1-[2,4-dihydroxy-6-methoxy-3-(3-methylbutyl)phenyl]-3-(4-  
hydroxyphenyl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



CC 10-5 (Microbial, Algal, and Fungal Biochemistry)

Section cross-reference(s): 11

IT 70-18-8, Glutathione, biological studies 94-41-7D, Chalcone,  
prenylated

derivs. 6754-58-1, Xanthohumol 16009-13-5, Hemin 68236-13-5  
115063-39-3 115063-40-6 250603-94-2 688360-14-7 864465-61-2  
864465-62-3

RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(antiplasmoidal activity of prenylated chalcone derivs. of hops  
(Humulus lupulus) and their influence on glutathione-dependent hemin  
degradation)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR  
THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L16 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:781478 CAPLUS

DOCUMENT NUMBER: 144:167259

TITLE: Brosimacutins J-M, four new flavonoids from  
Brosimum

acutifolium and their cytotoxic activity

AUTHOR(S): Takashima, Junko; Komiyama, Kanki; Ishiyama,  
Haruaki;

Kobayashi, Jun'ichi; Ohsaki, Ayumi

CORPORATE SOURCE: Research & Development Division, Mitsubishi Pharma  
Corporation, Yokohama, Japan

SOURCE: Planta Medica (2005), 71(7), 654-658

CODEN: PLMEAA; ISSN: 0032-0943

PUBLISHER: Georg Thieme Verlag  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Four new flavonoids, brosimacutins J-M (I-IV), were isolated from the bark of Brosimum acutifolium Huber together with a known flavan, brosimine A (5). The structures of compds. I-IV were elucidated by spectroscopic means. 27 Constituents of this plant including compds. 1-5 were evaluated

for their cytotoxic activity against murine leukemia P388 cells. Although

no compds. tested had any reversal effect on vincristine resistance, brosimacutins J-M were cytotoxic to vincristine-resistant P388 cells (IC50

4.4-19 µg/mL).

IT 874205-59-1P, Brosimacutin M

RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (brosimacutins J-M, four new flavonoids from Brosimum acutifolium

and

their cytotoxic activity)

RN 874205-59-1 CAPLUS

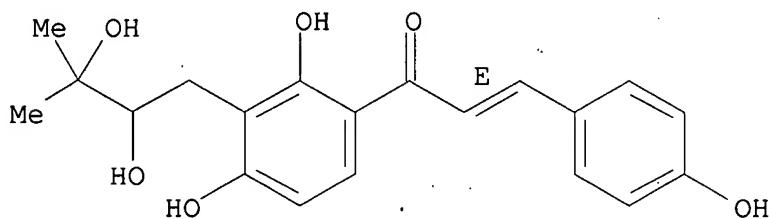
CN 2-Propen-1-one,

1-[3-(2,3-dihydroxy-3-methylbutyl)-2,4-dihydroxyphenyl]-3-(4-hydroxyphenyl)-, (2E)-(-) (9CI) (CA INDEX NAME)

Rotation (-).

Double bond geometry as shown.

Currently available stereo shown.



CC 11-1 (Plant Biochemistry)  
 Section cross-reference(s): 26

IT 874204-62-3P, Brosimacutin J 874205-55-7P, Brosimacutin K  
 874205-58-0P, Brosimacutin L 874205-59-1P, Brosimacutin M

10/581,034

RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
(brosimacutins J-M, four new flavonoids from Brosimum acutifolium  
and

their cytotoxic activity)

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:3740 CAPLUS

DOCUMENT NUMBER: 142:215204

TITLE: Prenylflavonoids and Phloroglucinol Derivatives  
from

Hops (*Humulus lupulus*)

AUTHOR(S): Zhao, Feng; Watanabe, Yuki; Nozawa, Hajime;  
Daikonna,

CORPORATE SOURCE: Akihiro; Kondo, Keiji; Kitanaka, Susumu  
Brewery Central Laboratories for Key Technology, Kirin

SOURCE: Co., Ltd., Kanagawa, 236-0004, Japan

Journal of Natural Products (2005); 68(1), 43-49  
CODEN: JNPRDF; ISSN: 0163-3864

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The Et acetate soluble fraction of hops (*Humulus lupulus*) showed potent inhibitory activity on the production of nitric oxide (NO) induced by a combination of LPS and IFN- $\gamma$ . Four known prenylflavonoids and a new prenylflavonoid, hulupinic acid, lupulone, and its six new derivs. were

were isolated from the active fraction. The structures were determined on the basis

of physiochem. properties and spectroscopic anal. Their inhibitory activities on the production of NO in macrophage RAW 264.7 cells were examined

IT 842121-72-6P

RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
(prenylflavonoids and phloroglucinol derivs. from *Humulus lupulus*)

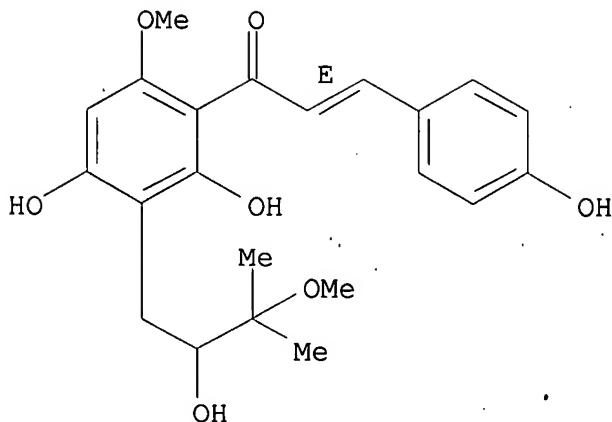
RN 842121-72-6 CAPLUS

CN 2-Propen-1-one,

1-[2,4-dihydroxy-3-(2-hydroxy-3-methoxy-3-methylbutyl)-6-methoxyphenyl]-3-(4-hydroxyphenyl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

Currently available stereo shown.



CC 11-1 (Plant Biochemistry)

Section cross-reference(s): 7, 26

IT 29366-64-1P, Lupulone E 613683-50-4P, Lupulone C 613683-51-5P,

Lupulone D 842121-72-6P 842121-73-7P, Lupulone A

842121-74-8P, Lupulone B 842121-75-9P, Lupulone F

RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(prenylflavonoids and phloroglucinol derivs. from Humulus lupulus)

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2004:965043 CAPLUS

DOCUMENT NUMBER: 141:415986

TITLE: Therapeutic agent for insulin-related disease

INVENTOR(S): Enoki, Tatsushi; Kobayashi, Eiji; Ogawa, Kinuko;

Kudo,

Yoko; Tanabe, Masashige; Sugiyama, Katsumi; Ohnogi, Hiromu; Sagawa, Hiroaki; Kato, Ikunoshin

PATENT ASSIGNEE(S): Takara Bio Inc., Japan

SOURCE: PCT Int. Appl., 289 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004096198	A1	20041111	WO 2004-JP6282	20040430
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,				

LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,  
 NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,  
 TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,  
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,  
 EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,  
 SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,  
 SN, TD, TG

EP 1623704	A1	20060208	EP 2004-730641	20040430
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1816328	A	20060809	CN 2004-80018286	20040430
US 2007092551	A1	20070426	US 2007-555017	20070103
JP 2007131637	A	20070531	JP 2007-21753	20070131
JP 2007186515	A	20070726	JP 2007-21740	20070131
PRIORITY APPLN. INFO.:			JP 2003-127517	A 20030502
			JP 2003-140821	A 20030519
			JP 2003-177280	A 20030620
			JP 2003-202118	A 20030725
			JP 2003-408213	A 20031205
			JP 2004-90656	A 20040325
			JP 2005-505944	A3 20040430
			WO 2004-JP6282	W 20040430

OTHER SOURCE(S): MARPAT 141:415986

AB Disclosed is a preventive or therapeutic agent for diseases  
accompanied by  
insulin level or insulin response disorder, characterized in that at  
least

one compound selected from the group consisting of chalcone compds.,  
acetophenone compds., coumarin compds., phthalide compds., derivs. of  
these and pharmacol. acceptable salts thereof is contained as an active  
ingredient. There are further provided an insulin-like agent; a food,  
beverage or feed; a promoter of glucose introjection in cells; and an  
agent capable of inducing differentiation to lipocytes. The agents are  
suitable for use in pharmaceuticals, foods, and/or feeds. For example,  
xanthoangelol was isolated from Angelica keiskei root, and in vitro  
tested

for its effect on adipocyte differentiation induction.

IT 791113-01-4P

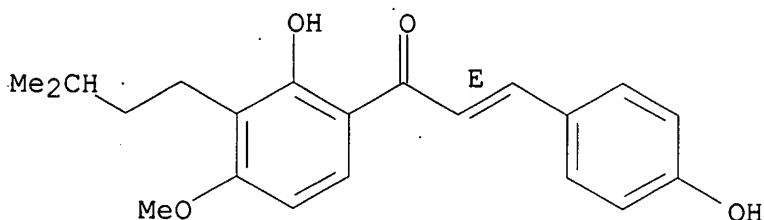
RL: FFD (Food or feed use); PAC (Pharmacological activity); SPN  
(Synthetic  
preparation); THU (Therapeutic use); BIOL (Biological study); PREP  
(Preparation); USES (Uses)  
(therapeutic agents for insulin-related disease containing chalcone

compds., acetophenone compds., coumarin compds., and/or phthalide compds.,)

RN 791113-01-4 CAPLUS

CN 2-Propen-1-one, 1-[2-hydroxy-4-methoxy-3-(3-methylbutyl)phenyl]-3-(4-hydroxyphenyl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IC ICM A61K031-121

ICS A61K031-222; A61K031-343; A61K031-341; A61K031-365; A61K031-351; A61K031-381; A61K031-366; A61K031-352; A61P043-00; A61P003-10; A61P003-08; A61P005-50; C07D493-08; C07D309-12; C07D311-32; C07C049-84; C07C049-835; C07C069-18; C07C069-157

CC 63-6 (Pharmaceuticals)

Section cross-reference(s): 1, 17, 18

IT 6272-43-1P, 3,4,2'-Trihydroxychalcone 20180-87-4P,

2'-Hydroxy-3'-geranyl-

4'-methoxyacetophenone 28437-37-8P 28448-85-3P, Bavachalcone  
31165-67-0P, 2'-Benzyl oxyacetophenone 37761-53-8P 63529-06-6P  
65786-15-4P 66549-80-2P 66549-83-5P 95832-45-4P 118062-82-1P  
126909-50-0P 162382-66-3P, Prostratol F 208659-72-7P

265652-88-8P,

Xanthoangelol G 352275-68-4P 352275-69-5P 791112-98-6P  
791113-00-3P 791113-01-4P 791113-02-5P 791113-03-6P  
791113-04-7P 791113-06-9P 791113-07-0P 791113-08-1P

791113-09-2P

791113-10-5P 791113-11-6P 791113-12-7P 791113-13-8P

791113-16-1P

791113-17-2P 791113-18-3P 791113-19-4P 791113-20-7P

791113-21-8P

791113-24-1P 791113-25-2P 791113-29-6P 791113-31-0P

791113-32-1P

791113-33-2P 791113-34-3P 791113-35-4P

RL: FFD (Food or feed use); PAC (Pharmacological activity); SPN

(Synthetic

preparation); THU (Therapeutic use); BIOL (Biological study); PREP  
(Preparation); USES (Uses)

(therapeutic agents for insulin-related disease containing chalcone  
compds., acetophenone compds., coumarin compds., and/or phthalide  
compds.,)

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR  
THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

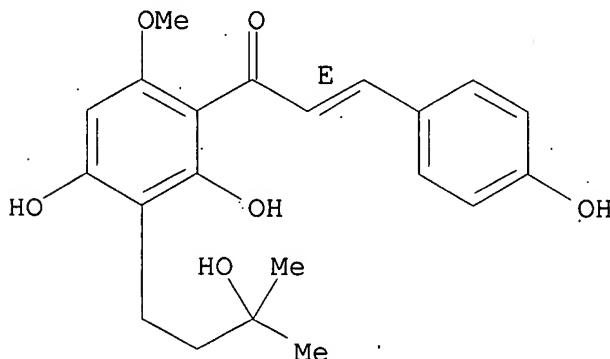
L16 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2004:1068127 CAPLUS  
 DOCUMENT NUMBER: 142:173331  
 TITLE: Estrogens and Congeners from Spent Hops (*Humulus lupulus*)  
 AUTHOR(S): Chadwick, Lucas R.; Nikolic, Dejan; Burdette, Joanna  
 CORPORATE SOURCE: E.; Overk, Cassia R.; Bolton, Judy L.; van Breemen, Richard B.; Froehlich, Roland; Fong, Harry H. S.; Farnsworth, Norman R.; Pauli, Guido F.  
 UIC/NIH Center for Botanical Dietary Supplements Research, Department of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, University of Illinois at Chicago, Chicago, IL, 60612, USA  
 SOURCE: Journal of Natural Products (2004), 67(12),  
 2024-2032  
 PUBLISHER: CODEN: JNPRDF; ISSN: 0163-3864  
 American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Estrogenicity-directed fractionation of a methanol extract of the strobiles of *Humulus lupulus* that had been extracted previously with supercrit. CO<sub>2</sub>, known as "spent hops", led to the isolation and identification of 22 compds. including 12 prenylated chalcones (1-8, 10-13), five prenylflavanones (14-17), 4-hydroxybenzaldehyde (18), sitosterol-3-O-β-glucopyranoside (19), humulinone (20), and cohumulinone (21). In addition, the prenylated chalcone xanthohumol C (9a) was obtained as a 6:1 mixture along with its 1'',2''-dihydro derivative (9b). Three new chalcones (4, 11, 12) and four previously unreported constituents of hops (5, 6, 9b, 13) are reported. The structures of the new compds. were determined through a combination of spectrometric techniques including 1D and 2D NMR, HRESIMS, and ESIMS-MS. Full 1H NMR spin system analyses were performed to characterize the higher-order glucopyranosyl, prenyl, and chalcone B-ring spectra of the isolates. The principle estrogen 8-prenylnaringenin (15) from hops is an artifact formed along with its positional isomer 6-prenylnaringenin (16) through the spontaneous isomerization of the pro-estrogenic chalcone DMX (7).  
 IT 688359-98-0P, Xanthohumol H 832078-79-2P, Xanthohumol G  
 RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (estrogens and congeners from *Humulus lupulus*)

10/581,034

RN 688359-98-0 CAPLUS

CN 2-Propen-1-one, 1-[2,4-dihydroxy-3-(3-hydroxy-3-methylbutyl)-6-methoxyphenyl]-3-(4-hydroxyphenyl)-, (2E)- (CA INDEX NAME)

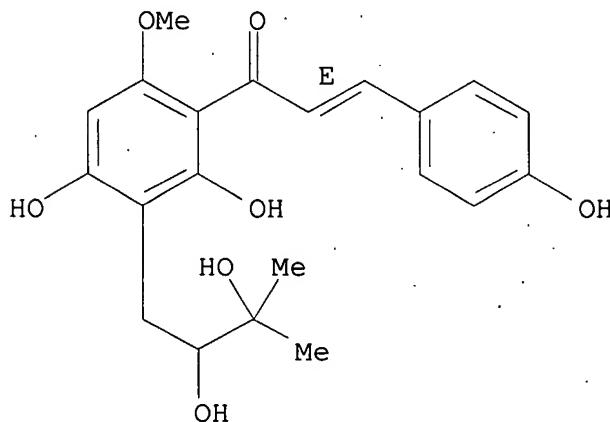
Double bond geometry as shown.



RN 832078-79-2 CAPLUS

CN 2-Propen-1-one, 1-[3-(2,3-dihydroxy-3-methylbutyl)-2,4-dihydroxy-6-methoxyphenyl]-3-(4-hydroxyphenyl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



CC 11-1 (Plant Biochemistry)

Section cross-reference(s): 26

IT 250603-94-2P 688359-98-0P, Xanthohumol H 688360-06-7P,  
Xanthohumol I 831227-04-4P 831227-05-5P, Desmethylxanthohumol B  
831227-06-6P, Desmethylxanthohumol J 832078-79-2P, Xanthohumol G  
RL: BSU (Biological study, unclassified); NPO (Natural product  
occurrence); PRP (Properties); PUR (Purification or recovery); BIOL  
(Biological study); OCCU (Occurrence); PREP (Preparation)  
(estrogens and congeners from Humulus lupulus)

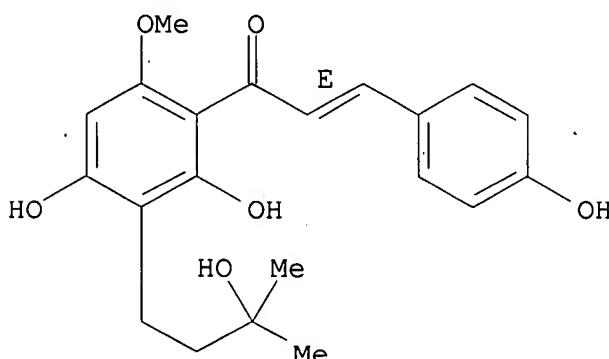
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR  
THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L16 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2004:173234 CAPLUS  
 DOCUMENT NUMBER: 140:399280  
 TITLE: Xanthohumol metabolites in feces of rats  
 AUTHOR(S): Nookandeh, Aslieh; Frank, Norbert; Steiner, Frank;  
 Ellinger, Renate; Schneider, Bernd; Gerhauser,  
 Clarissa; Becker, Hans  
 CORPORATE SOURCE: Institute for Pharmacognosy and Analytical  
 Phytochemistry, University of the Saarland,  
 Saarbrucken, 66041, Germany  
 SOURCE: Phytochemistry (Elsevier) (2004), 65(5), 561-570  
 CODEN: PYTCAS; ISSN: 0031-9422  
 PUBLISHER: Elsevier Science B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Xanthohumol (1), isolated from hop, was fed to rats in a dose of 1000  
 mg kg<sup>-1</sup> body weight. The feces of the animals were collected after 24 and  
 48 h and analyzed for metabolites of 1. Approx. 89% of the recovered  
 flavonoid-compds. consisted of unchanged 1. Sixteen metabolites and  
 six previously known metabolites were isolated and characterized by  
 coupling techniques (HPLC-NMR, HPLC-MS and HPLC-DAD). Their structures were  
 elucidated by spectroscopic methods, especially using NMR  
 spectroscopy. Twenty metabolites had a modified chalcone structure and two metabolites were  
 flavanone derivs.  
 IT 688359-98-0  
 RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (xanthohumol metabolites in feces of rats)  
 RN 688359-98-0 CAPLUS  
 CN 2-Propen-1-one, 1-[2,4-dihydroxy-3-(3-hydroxy-3-methylbutyl)-6-  
 methoxyphenyl]-3-(4-hydroxyphenyl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



CC 1-2 (Pharmacology)  
 IT 6754-58-1, Xanthohumol 70872-29-6, Isoxanthohumol 189299-05-6  
 250603-94-2 274675-25-1 688359-98-0 688359-99-1  
 688360-00-1 688360-01-2 688360-02-3 688360-03-4 688360-04-5  
 688360-05-6 688360-06-7 688360-07-8 688360-08-9 688360-09-0  
 688360-10-3 688360-11-4 688360-12-5 688360-13-6 688360-14-7  
 688360-15-8  
 RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (xanthohumol metabolites in feces of rats)  
 REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR  
 THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

L16 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2003:363073 CAPLUS  
 DOCUMENT NUMBER: 139:332335  
 TITLE: Inhibitors of nitric oxide production from hops  
 (Humulus lupulus L.)  
 AUTHOR(S): Zhao, Feng; Nozawa, Hajime; Daikonna, Akihiro;  
 Kondo,  
 Keiji; Kitanaka, Susumu  
 CORPORATE SOURCE: Central Laboratories for Key Technology, Kirin  
 Brewery  
 Co., Ltd., Kanagawa, 236-0004, Japan  
 SOURCE: Biological & Pharmaceutical Bulletin (2003), 26(1),  
 61-65  
 CODEN: BPBLEO; ISSN: 0918-6158  
 PUBLISHER: Pharmaceutical Society of Japan  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Nitric oxide (NO) plays an important role in many inflammatory responses  
 and is also involved in carcinogenesis. In the present study, we investigated the inhibitory effect of exts. from Humulus lupulus L. on both the production of NO and the expression of inducible NO synthase (iNOS) in mouse macrophage RAW 264.7 cells. The production of NO was induced by a combination of lipopolysaccharide (LPS) and IFN- $\gamma$ , and determined by Griess assay. The expression of iNOS was detected by Western blotting. The LPS/IFN- $\gamma$ -induced production of NO and expression of iNOS were significantly inhibited by the Et acetate soluble fraction of Humulus lupulus L. Through bioactivity guided fractionation, humulene, five chalcones, 2,2-di-(3-methyl-2-butyleyl)-4,5-dihydroxy- cyclopent-4-en-1,3-dione, lupulone and three of its derivs. were isolated from the Et acetate soluble fraction. The chalcones, including xanthohumol, significantly inhibited the production of NO by suppressing the expression of iNOS.

IT 613683-49-1P

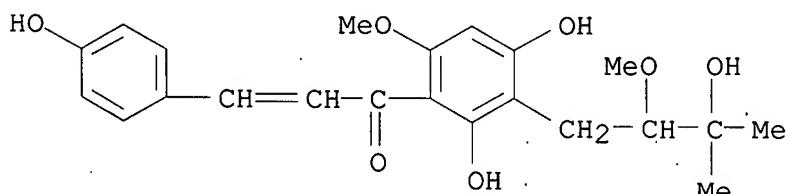
RL: ADV (Adverse effect, including toxicity); NPO (Natural product occurrence); PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)

(preparation and structure activity of nitric oxide inhibitors extracted from hops)

RN 613683-49-1 CAPLUS

CN 2-Propen-1-one,

1-[2,4-dihydroxy-3-(3-hydroxy-2-methoxy-3-methylbutyl)-6-methoxyphenyl]-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



CC 1-3 (Pharmacology)

Section cross-reference(s): 11

IT 94-41-7P, Chalcone 468-28-0P 1891-42-5P 6753-98-6P, Humulene 6754-58-1P, Xanthohumol 29366-64-1P 102448-00-0P 189308-10-9P, Xanthohumol B 274675-25-1P, Xanthohumol D 613683-49-1P 613683-50-4P 613683-51-5P

RL: ADV (Adverse effect, including toxicity); NPO (Natural product occurrence); PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)

(preparation and structure activity of nitric oxide inhibitors extracted from hops)

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1989:614230 CAPLUS

DOCUMENT NUMBER: 111:214230

TITLE: Preparation and formulation of chalcone derivatives as aldose reductase inhibitors

INVENTOR(S): Chin, Masao; Sato, Shunji; Hosaka, Kunio; Mihashi, Hiroshi

PATENT ASSIGNEE(S): Tsumura and Co., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 44 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01013019	A	19890117	JP 1987-142166	19870609
PRIORITY APPLN. INFO.:			JP 1987-142166	19870609

OTHER SOURCE(S): MARPAT 111:214230

GI For diagram(s), see printed CA Issue.

AB Chalcone compds. (I; X = Y = H, XY = bond; R1 = OH, AcO, HO<sub>2</sub>CCH<sub>2</sub>O, MeO<sub>2</sub>CCH<sub>2</sub>O; R2 = isoprenyl isopentyl, Pr, H; R3 = OH, MeO; R4, R5 = H, OH, MeO) effective reductase inhibitors, are prepared Condensation of ketone II

(preparation given) with aldehyde III (preparation given) in KOH-EtOH gave 78.3%

unsatd. ketone IV which was hydrogenated over 5% Pd-C to give 97.3% saturated

ketone. Hydrolysis of the saturated ketone in HCl-MeOH gave 39.0% I (X = Y =

H, R1 = R3 = R5 = OH; R2 = R4 = H) (V) which (5.0 %) was formulated with

150 mL polysorbate-80 and 4.85 L sterilized saline to make injection vials

containing 10 mg V each. V showed 99.0% inhibition of aldose reductase in rat

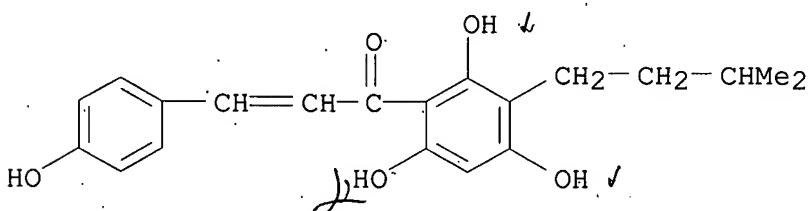
lens at 10-4M.

IT 112772-81-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as aldose reductase inhibitor)

RN 112772-81-3 CAPLUS

CN 2-Propen-1-one, 3-(4-hydroxyphenyl)-1-[2,4,6-trihydroxy-3-(3-methylbutyl)phenyl]- (9CI) (CA INDEX NAME)



IC ICM A61K031-12

ICS A61K031-22; A61K031-235; C12N009-99

ICA C07C049-82; C07C049-84; C07C069-12; C07C069-708; C07C069-94

CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 1, 63IT 60-82-2P 21849-70-7P 23130-26-9P 57765-66-9P 73692-51-0P  
100634-10-4P 112772-63-1P 112772-71-1P 112772-73-3P

112772-74-4P

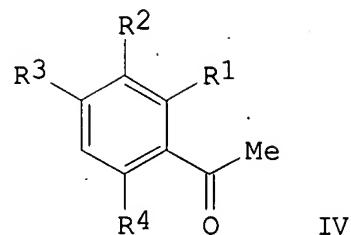
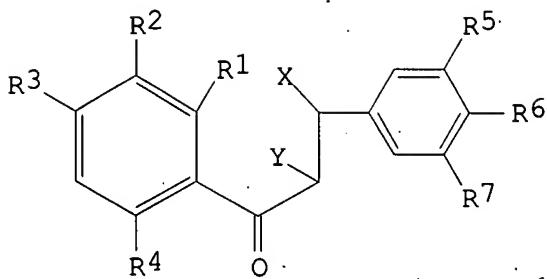
112772-79-9P 112772-80-2P 112772-81-3P 112772-82-4P  
 118055-99-5P 118056-04-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, as aldose reductase inhibitor)

L16 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1989:23539 CAPLUS  
 DOCUMENT NUMBER: 110:23539  
 TITLE: Antiulcer agents containing chalcone derivatives as effective ingredients and novel chalcone derivatives  
 INVENTOR(S): Komazawa, Yukio; Takeda, Shigehumi; Hosaka, Kunio; Mitsuhashi, Hiroshi; Watanabe, Toshihiko  
 PATENT ASSIGNEE(S): Tsumura Juntendo, Inc., Japan  
 SOURCE: PCT Int. Appl., 256 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

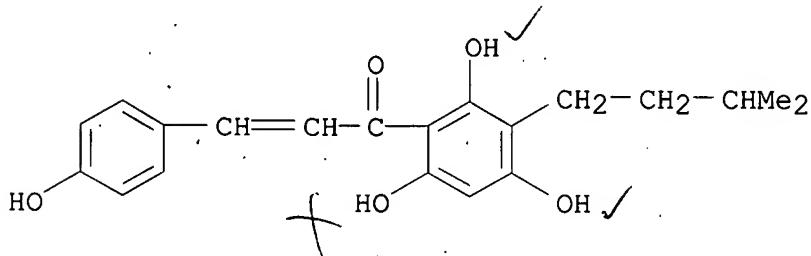
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8804288	A1	19880616	WO 1987-JP973	19871212
W: HU, KR, US RW: AT, BE, CH,	DE, FR, GB, IT, NL			
JP 63150241	A	19880622	JP 1986-294952	19861212
JP 01042422	A	19890214	JP 1987-198197	19870810
EP 292576	A1	19881130	EP 1988-900102	19871212
R: AT, BE, CH,	DE, FR, GB, IT, LI, NL			
HU 52026	A2	19900628	HU 1988-311	19871212
HU 203515	B	19910828		
US 5106871	A	19920421	US 1991-733003	19910719
US 5234951	A	19930810	US 1991-797063	19911125
PRIORITY APPLN. INFO.:			JP 1986-294952	A 19861212
			JP 1987-198197	A 19870810
			WO 1987-JP973	W 19871212
			US 1988-237850	B1 19880720
			US 1989-436088	B1 19891109
			US 1991-733003	A3 19910719

OTHER SOURCE(S): MARPAT 110:23539  
 GI



AB      Ulcer inhibitors containing chalcone derivs. I (X, Y = H or XY = bond; R1 = OH, AcO, HO<sub>2</sub>CCH<sub>2</sub>O, MeO<sub>2</sub>CCH<sub>2</sub>O; R2 = H, isoprenyl, isopentyl, Pr; R3 = OH, Me; R4 = H, OH, MeO; R5 = H, OH, MeO, isopentyl; R6 = OH, MeO, MeO<sub>2</sub>C; R7 = H, MeO) (II) and chalcone derivs. I (X, Y, R2, R3, R4, R6, R7 as specified above; R1 = OH, HO<sub>2</sub>CCH<sub>2</sub>O; R5 = H, OH, MeO; but R6 = MeO when R5 = OH, R6 = OH when R5 = MeO; etc.) (III) are prepared To a mixture of an acetophenone IV (R1 = R3 = R4 = OH, R2 = H) and K<sub>2</sub>CO<sub>3</sub> in THF was added dropwise ClCH<sub>2</sub>CH:CMe<sub>2</sub> and the mixture was further stirred 2 days to give 34.0% IV (R1 = R3 = R4 = OH, R2 = Me<sub>2</sub>C:CHCH<sub>2</sub>) which was stirred 1 h with (Me<sub>2</sub>CH)<sub>2</sub>EtN in THF and to the resultant stirred mixture was added dropwise ClCH<sub>2</sub>OMe to give IV (R1 = OH; R3 = R4 = MeOCH<sub>2</sub>O; R2 = Me<sub>2</sub>C:CHCH<sub>2</sub>) (V). V and 3-methoxy-4-methoxymethoxybenzaldehyde in EtOH were condensed by addition of saturated KOH in aqueous EtOH at 0° and stirring the resultant mixture 15 h at room temperature to give 57.0% diphenylpropanone I (XY = bond, R1 = OH, R2 = Me<sub>2</sub>C:CHCH<sub>2</sub>, R3 = R4 = R6 = MeOCH<sub>2</sub>O, R5 = MeO, R7 = H) which was hydrogenated over 5 % Pd-C to give 93.8% diphenylpropanone I (X = Y = R7 = H, R1 = OH, R2 = isopentyl, R3 = R4 = R6 = MeOCH<sub>2</sub>O, R5 = MeO) which was hydrolyzed to give 50.9% chalcone derivative III (X = Y = R7 = H, R1 = R3 = R4 = R6 = OH, R2 = isopentyl, R5 = MeO). At 100 mg/kg, p.o., in rats, a similarly prepared chalcone derivative I (X = Y = H, R1 = HO<sub>2</sub>CCH<sub>2</sub>O, R2 = isopentyl, R3 = R6 = MeO, R4 = R5 = R7 = H) (VI) gave 93% inhibition against rat stomach ulcer induced by 1 mL EtOH, p.o. At >1 g/kg, p.o., II and/or III caused no death in rats. An injection liquid as an ulcer inhibitor was formulated by mixing 7.5 g VI, 150 mL polysorbate 80, and

4.85 L physiolog. saline solution  
 IT 112772-81-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, as ulcer inhibitor)  
 RN 112772-81-3 CAPLUS  
 CN 2-Propen-1-one, 3-(4-hydroxyphenyl)-1-[2,4,6-trihydroxy-3-(3-methylbutyl)phenyl]- (9CI) (CA INDEX NAME)



IC C07C049-82; C07C049-84; C07C059-70; C07C069-21  
 CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 Section cross-reference(s): 1, 63  
 IT 60-82-2P 13745-20-5P 73692-51-0P 112772-63-1P 112772-65-3P  
 112772-66-4P 112772-67-5P 112772-69-7P 112772-71-1P  
 112772-73-3P  
 112772-74-4P 112772-76-6P 112772-78-8P 112772-79-9P  
 112772-80-2P  
 112772-81-3P 112772-82-4P 118055-95-1P 118055-96-2P  
 118055-98-4P 118056-01-2P 118056-04-5P 118056-07-8P  
 118056-08-9P  
 118056-09-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, as ulcer inhibitor)

L16 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN

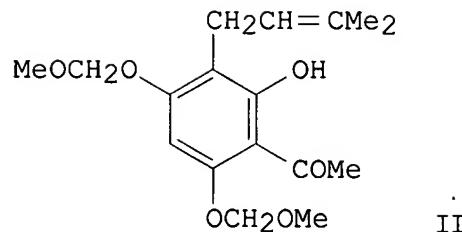
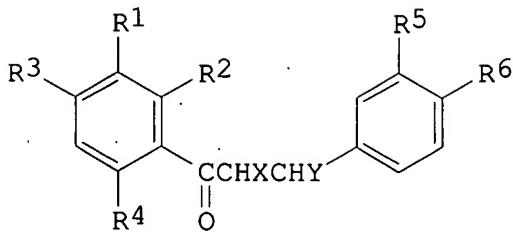
ACCESSION NUMBER: 1988:74984 CAPLUS  
 DOCUMENT NUMBER: 108:74984  
 TITLE: Preparation of chalcone derivatives as  
 hyaluronidase

INVENTOR(S): Hosaka, Kunio; Chin, Masao; Mihashi, Hiroshi  
 PATENT ASSIGNEE(S): Tsumura Juntendo, Inc., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 34 pp.  
 CODEN: JKXXAF

DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62185037	A	19870813	JP 1986-26775	19860212
PRIORITY APPLN. INFO.:			JP 1986-26775	19860212

GI



AB Chalcone derivs. (I; R<sub>1</sub> = isoprenyl, isopentyl, H; R<sub>2</sub> = H, OH, AcO, HO<sub>2</sub>CCH<sub>2</sub>O, MeO<sub>2</sub>CCH<sub>2</sub>O; R<sub>1</sub> = OH, MeO, PhCH<sub>2</sub>O; R<sub>4</sub> = H, OH, MeO, PhCH<sub>2</sub>O; R<sub>5</sub>

= H, OH, MeO, Me<sub>2</sub>CHCH<sub>2</sub>; R<sub>6</sub> = OH, MeO; X, Y = H, XY = bond), useful as hyaluronidase inhibitors, are prepared Condensation of acetophenone derivative

II with p-MeOCH<sub>2</sub>OC<sub>6</sub>H<sub>4</sub>CHO over MeONa-MeOH gave 88.2% chalcone derivative I (R<sub>1</sub>

= isoprenyl, R<sub>2</sub> = OH, R<sub>3</sub> = R<sub>4</sub> = R<sub>6</sub> = MeOCH<sub>2</sub>O, R<sub>5</sub> = H, XY = bond), which was refluxed in HCl-MeOH to give 27% hydroxy derivative I (R<sub>1</sub> = isoprenyl; R<sub>2</sub>

= R<sub>3</sub> = R<sub>4</sub> = R<sub>6</sub> = OH; R<sub>5</sub> = H; XY = bond), which inhibited hyaluronidase by

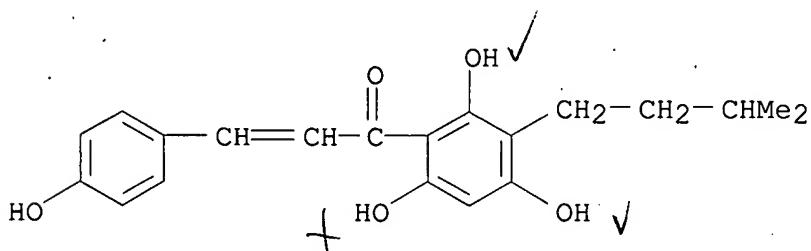
88.3% at 1.0 g/mL.

IT 112772-81-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as hyaluronidase inhibitor)

RN 112772-81-3 CAPLUS

CN 2-Propen-1-one, 3-(4-hydroxyphenyl)-1-[2,4,6-trihydroxy-3-(3-methylbutyl)phenyl]- (9CI) (CA INDEX NAME)



IC ICM C07C049-83

ICS C07C049-84; C07C059-70; C07C069-14

ICA A61K031-12; A61K031-19; A61K031-22; C12N009-99

CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 1

IT 57765-66-9P 100634-10-4P 112772-73-3P 112772-74-4P 112772-75-5P  
112772-76-6P 112772-77-7P 112772-78-8P 112772-79-9P

112772-80-2P

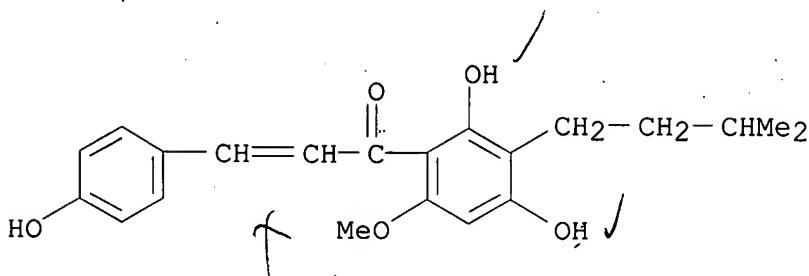
112772-81-3P 112772-82-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as hyaluronidase inhibitor)

L16 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1961:105840 CAPLUS  
 DOCUMENT NUMBER: 55:105840  
 ORIGINAL REFERENCE NO.: 55:19917e-i  
 TITLE: An experimental contribution to the study of the isomerization of  $\alpha,\beta$  and  $\beta,\gamma$ -unsaturated ketones  
 AUTHOR(S): Anteunis, M.  
 SOURCE: Verhandel. Koninkl. Vlaam. Acad. Wetenschap., Belg., K1. Wetenschap. (1960), 22(No. 64), 1-86  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB The mechanism of the isomerization of  $\alpha,\beta$  and  $\beta,\gamma$ -unsatd. ketones in the presence of bases as described by Ingold, et al. (CA 20, 2823), was verified when the hindered 1-phenyl-2,2,3-trimethylbut-3-en-1-one, b1 90°, did not isomerize in 5N NaOH in aqueous alc. With its explanation of a pos.  $\beta$ -C this mechanism agreed also with the observation of OH addns. to  $\alpha,\beta$ -unsatd. ketones sometimes followed by a "retrograde aldol condensation." In this work  $\beta$ -addition converted chalcones to flavanones, but only if the chalcones had multiple phenolic OH groups. 4-Benzylxy-2',4'-dihydroxy-6'-methoxychalcone (I), m. 216-18°, was treated with 5% KOMe solution for 5 min. After evaporation of the solvent, unreacted I was removed by hot extraction with Et<sub>2</sub>O, and the residue was recrystd. from aqueous Me<sub>2</sub>CO to give the corresponding flavanone, 2-(p-benzylxyphenyl)-5-methoxy-7-hydroxy-4-chromone (II), m. 202-3°. At the m.p. II reverted to I. Xanthohumol (CA 51, 14706a; 52, 7243d) in 2-5% NaOH solution gave the expected flavanone, isoxanthohumol, m. 198°, in 95% yield. Attempts to repeat this ring closure with 2'-hydroxychalcone (isomeric mixture), m. 100-45°, and 2'-hydroxy-5'-methylchalcone, m. 142-3°, failed. An attempt to prepare bicoumarinyl by the method of Dyson and Fittig [Ann. 225, 275(1889)] from salicylaldehyde and Na succinate gave a 15% yield with a balance of 1,4-bis(o-hydroxyphenyl)butadiene-2,3-dicarboxylic anhydride, m. 330° (PhMe); the separation was carried out in CHCl<sub>3</sub>. An analogous reaction with o-methoxybenzaldehyde produced 1,4-bis(o-methoxyphenyl)butadiene, m. 118° (C<sub>5</sub>H<sub>6</sub>-isooctane), in 8.5% yield and 1,4-bis(o-methoxyphenyl)butadiene-2-carboxylic acid, m. 179-80° (C<sub>6</sub>H<sub>5</sub>-isooctane).  
 IT 102447-96-1P, Chalcone, 2',4,4'-trihydroxy-3'-isopentyl-6'-methoxy-  
 RL: PREP (Preparation)  
 (preparation of).  
 RN 102447-96-1 CAPLUS

10/581,034

CN Chalcone, 2',4,4'-trihydroxy-3'-isopentyl-6'-methoxy- (6CI) (CA INDEX  
NAME)



CC 10G (Organic Chemistry: Heterocyclic Compounds)

IT 708-53-2P, Acetophenone, 2',3'-dihydroxy-4'-methoxy- 2243-53-0P,  
3-Butenoic acid, 4-phenyl- 4168-01-8P, 3-Butenoic acid,  
2,2,3-trimethyl-

13389-88-3P, Succinic acid, ( $\alpha$ -hydroxybenzyl)-,  $\gamma$ -lactone  
23783-79-1P, 3,3'-Bicoumarin 38641-96-2P, 1,3-Butadiene,  
1,4-bis(o-methoxyphenyl)- 96169-02-7P, Propiophenone,  
2',4'-dihydroxy-3-(p-hydroxyphenyl)-3'-isopentyl-6'-methoxy-  
100612-23-5P, 2-Pentenophenone, 2'-hydroxy-4,4'-dimethyl-

101109-98-2P,

3-Butenoic acid, 4-phenyl-, phenyl ester 102447-96-1P, Chalcone,  
2',4,4'-trihydroxy-3'-isopentyl-6'-methoxy- 102448-00-0P,

Propiophenone,

2',4'-dihydroxy-3-(p-hydroxyphenyl)-6'-methoxy-3'-(3-methyl-2-butenyl)-  
109690-85-9P, Cinnamic acid, o-methoxy- $\alpha$ -(o-methoxystyryl)-  
111385-02-5P, Succinic anhydride, disalicylidene- 112599-37-8P,  
Flavanone, 4'-(benzyloxy)-7-hydroxy-5-methoxy- 852638-51-8P, Flavone,  
4',7-dihydroxy-5-methoxy-8-(3-methyl-2-butenyl)- 857402-56-3P,

Flavone,

4',7-dihydroxy-8-isopentyl-5-methoxy-

RL: PREP (Preparation)  
(preparation of)

=> log y

COST IN U.S. DOLLARS

SINCE FILE  
ENTRY

TOTAL

SESSION

FULL ESTIMATED COST

96.31

451.96

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE  
ENTRY

TOTAL

SESSION

CA SUBSCRIBER PRICE

-13.26

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